Indian J. Phys. **70A** (1), 69 – 79 (1996)

IJP A
— an international journal

Raising collectivity in the shell model

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Abstract : The primary concept in the nuclear shell model is the central mean field operating on each nucleon. This itself is a collective feature of the nucleus, and all collective dynamics flows from this. Hartree-Fock method offers a direct way to generate such a central field, but generally this results in loss of spherical symmetry for the single particle wave functions. However, one can treat the HF field as a basis for a deformed shell model. A limited amount of configuration mixing in this basis space can provide excellent approximation to a full spherical shell model calculation, and in addition provide a direct physical insight. The method of DCM will be described in detail, and some recent applications to bromine isotopes will be discussed.

Keywords : Nuclear shell model, collective property

PACS No. : 21.60. Cs

1. Introduction

The nucleus presents to its devotees a variety of different facets depending upon the probes used to explore it. We make nuclear models by comparing the facet thus revealed with some manybody system familiar to us. Thus different nuclear models treat the nucleus as a crystal, a liquid drop, a rotating top, a Fermi gas *etc*. An interesting field of study has always been to look for connections or bridges between these different models, especially in terms of some universal microscopic theory. The nuclear shell model offers such a wide microscopic basis. The central concept in the shell model is the mean field which operates on each individual nucleon, and within which they move almost independently. This mean field itself is a collective concept and its shape and dynamics can be studied in a microscopic framework. This provides a simple and direct route to study collective properties of nuclei in a microscopic shell model approach.

An early formalism to generate a mean field in a complex interacting many body system was suggested by Hartree and extended by Fock to take into account the symmetry

of the wave functions for identical particles. The Hartree-Fock approach was used very successfully to describe rotational spectra of well deformed nuclei [1,2]. However, in early applications it was considered essential to have a large energy gap in the HF spectrum between occupied and unoccupied states, as otherwise the HF solution would be unstable to pairing excitations. This inhibited a wider use of the HF formalism.

The HF method uses a variational approach which minimises the ground state energy of a nucleus. A constraint imposed in the interest of simplicity is that the ground state wavefunction is a single Slater determinant. With this constraint the HF determines the single particle wavefunctions and energies which will lead to the lowest energy for the Slater determinant (many-body) wavefunction constructed out of these single particle wavefunctions. The price one has to pay for this constraint is that to obtain a reasonable energy of the ground state one has to give up the spherical symmetry. Although the Hamiltonian used is spherically symmetric, the single particle wavefunctions (and consequently the Slater determinant constructed out of them) do not have a good angular momentum quantum number. They can be visualised as if arising from a deformed mean field or a central potential. Keeping axial symmetry often gives good results, but sometimes one has to abandon even that and resort to a triaxial central potential. While on the one hand, this leads to the necessity of using projection operators [2] to obtain states of good angular momenta, and their energies for comparison with experimental data, the conceptual advantage in the other hand is that the shapes and deformations and their variation with different nuclear parameters emerge automatically from the HF approach. Thus the HF method provides a direct and fruitful insight into the collective dynamics of nuclei.

Calculations in the spherical shell model basis also do reproduce the collective properties of nuclei, *e.g.* the rotational spectrum and enhanced E2 transitions in ^{20}Ne [3]. However, to obtain good results one must mix a very large mumber of configurations, *e.g.* about 50 in case of ^{20}Ne. In the HF approach, a single intrinsic configuration will give the entire rotational band and its properties. To reproduce collective properties for ^{22}Ne spectrum, one needs to mix more than 500 configurations !

As developed in earlier days (in 1960's) HF method had two major problems. One, as we discussed earlier, was the lack of adequately large gaps in most nuclei, which necessitates taking into account pairing interactions. It is a commonly accepted statement that HF method does not take into account a vital part of the nuclear Hamiltonian *viz.* pairing. One way to remedy this is the Hartree-Fock-Bogoliubov (HFB) approach. The other problem with HF method was that one often finds several different solutions (or configurations) which give nearly degenerate energies. Which shape or configuration does the nucleus choose ?

It should be obvious at this stage that it would be wrong to interprete the Hartree-Fock method in a very restrictive manner, *viz.* that it gives a single Slater determinantal wave function from which to determine nuclear properties. Our approach should be that the HF leads to a mean field which gives a scheme of single particle wavefunctions and their energies *etc.* which can be used as a shell model basis-of course, a deformed shell model.

The HF spectrum can be used to generate a configuration space in terms of which the nuclear properties can be described just as we did in the spherical shell model.

2. Deformed shell Model

My own acquaintance with the HF method was only begun around 1970. Prior to that considerable contributions to this field had already been made by groups at Saha Institute of Nuclear Physics and Tata Institute of Fundamental Research, but I was blissfully ignorant of all that. I was led to the idea of using HF as a means of generating a deformed shell model from the reading of the classic paper of Ripka [1] and then an interesting note by Macfarlane and Shukla [4]. They asked : if we start with a deformed shell model as given by HF, how much and what kind of configuration mixing one must take into account to reproduce the corresponding spherical shell model spectra for ^{20}Ne and ^{22}Ne ? Actually, ^{20}Ne is already an almost perfect rotational case, and ^{22}Ne is nearly so. With my shell model background I was immediately attracted to this idea. It was known at the time that the low-lying states of ^{24}Ne appear to have a vibrational-like spectrum. While a HF basis can be expected to generate quickly a rotational spectrum as in ^{20}Ne and ^{22}Ne, it would be really interesting to see if it can lead to a vibration-like spectrum. Dr. S C K Nair and Dr. S B Khadkikar, who were already experts in this field quickly tested this idea [5], with further elaboration by Kulkarni and Khadkikar [6], and it was shown that as against more than 500 configurations needed in the spherical shell model basis, less than a dozen configurations would suffice to explain the experimental data in the deformed basis. Calculations with a few configurations in deformed shell model (DSM) basis can generate collective features in nuclei that would need hundreds of configurations in the spherical basis. This has become very apparent in medium and heavy nuclei.

For the last two decades we have carried out a large scale program of studying collective dynamics of nuclei in the DSM approach with applications to many nuclei in *d-s* shell, *f-p* shell and $f_{5/2} - p_{3/2} - p_{1/2} - g_{9/2}$ shell region. Elsewhere our colleagues have also applied this approach to heavier nuclei *e.g.*Hg, rare-earth nuclei, Xe *etc.* I will skip these details [7].

The DSM approach has many advantages. For most nuclei, the spherical shell model requires such a large number of configurations to be mixed that a calculation of this magnitude is beyond the capacity of most computers available to us here even today. In the DSM approach the number of configurations needed are of the order of 10-20 only. This is because already the DSM scheme generated by a HF calculation incorporates a large part of the nucleon-nucleon interaction. It is very easy to take into account pairing correlations. If we deal with axially symmetric solutions, one can include several excited $K = 0$ configurations which differ from the ground state by appropriate two particle two hole pair excitations, *e.g.*

$$|K = 0\rangle = \mathrm{Cl}^{+}_{k_2}\ \mathrm{Cl}^{+}_{\bar{k}_2}\ \mathrm{Cl}_{k_1}\ \mathrm{Cl}_{\bar{k}_1}\ |0\rangle$$

where the bar on the projection quantum number k denotes a time-reversed state. One can also simulate triaxiality in the axially symmetric solutions by mixing ground state $K = 0$

with excited configurations with $K = 2$, $K = 4$ *etc.* [8]. In fact, Bhatt [9] has pointed out that even a band of states projected from a single intrinsic HF state, gives results very close to those of a triaxial rotor model. By including suitable configurations with high K value, one can easily generate high-spin states [10]. By a simple inspection of the HF-DSM scheme one can identify and include configurations with small and/or large deformations, and thus obtain shape coexistence, band crossing, rotation alignment and many such observed properties. The most obvious advantage is that the physics becomes easily transparent. Collective band structures are identified in a straightforward manner. One can see the microscopic structure of such bands at once. It is useful at this stage to note that the way we handle DSM, in a limited configuration space, leads to a very good approximation to the spherical shell model.

3. Formalism

It may be useful to review briefly the mathematical steps involved in this DSM approach. The initial step as in the spherical shell model is to choose in the spherical basis a configuration space for active nucleons. The single particle orbits in this space have harmonic oscillator wavefunctions and the single particle energies are chosen on the basis of appropriate experimental data. Then a Hartree-Fock calculation is done for a given number of neutrons and protons in this space. The calculation involves a specified nucleon-nucleon interaction. We have generally imposed the constraint of axial symmetry, since as discussed earlier, one could simulate non-axial-symmetry in this framework easily, whereas projection of good J states from non-axially-symmetric solutions becomes very difficult. The HF gives an intrinsic configuration — the DSM basis — with the lowest energy. We now have a set of DSM single particle states (characterised by k quantum numbers) and their energies — DSM configuration space. In addition to the lowest energy configuration, one can choose several other configurations in this space with appropriate properties. This choice has to be guided essentially by the physics one wants to extract from the calculations. For each of these additional configurations, we carry out a constrained or tagged HF to determine for them, self-consistently the energy, quadrupole moment, single particle spectrum *etc.* We have now for each configuration a Slater determinant Ψ_K. To return to experimental data, we project out from each a band of states of good angular momenta,

$$\Psi_J[K] = P_J \left| \Psi_K \right\rangle$$

Obviously, the states $\Psi_J[K]$ projected from different intrinsic states are not orthogonal to each other. Hence to diagonalise the Hamiltonian in the space of these $\Psi_J[K]$, we construct the overlap matrix and the Hamiltonian matrix.

$$O^J_{KK'} = \left\langle \Psi_J\,[K] \middle| \Psi_J\,[K'] \right\rangle$$

and

$$H^J_{KK'} = \left\langle \Psi_J\,[K] \middle| H \middle| \Psi_J\,[K'] \right\rangle$$

Finally, we solve the elgenvalue problem

$$\sum_{K'} \left(H^J_{KK'} - EO^J_{KK'}\right)C_{K'} = 0$$

for each J. This yields a set of states

$$\Psi_J = \sum_K C_K \Psi_J(K)$$

and their energies. Calculations of other properties of these states are straightforward. One is now ready to compare the results of above calculations with experimental data. The mathematics involved is all standard, and is described by Dhar *et al* [11].

4. Results for bromine isotopes

To illustrate the working of this DSM approach, I will consider some of the odd-even isotopes of bromine. Br has 35 protons. We have earlier discussed the structure of isotopes with N = 42, 44 and 46 [12]. In future we hope to extend the studies to neutron-rich isotopes with N ≥ 50. In this paper we consider the proton-rich isotopes with N = 36, 38 and 40.

The mass region A = 70-90 is being intensively studied by nuclear structure physicists today. The nuclei-far-from-stability in this region show fascinating unexpected properties. The spherical configuration space for active nucleons is taken to consist of $f_{5/2}$, $p_{3/2}$, $p_{1/2}$ and $g_{9/2}$ states with ^{56}Ni as a closed inert core. The single particle energies of these states are taken as 0.78, 0.00, 1.08 MeV for the first three (from data on ^{57}Ni) and 4.5 MeV for the $g_{9/2}$ state in view of our past experience [13]. The details of the spectral and other properties will be somewhat sensitive to these single particle energies as we shall discuss - but not the general characteristics. An effective nucleon-nucleon interaction in this space has been derived by Kuo and modified by Ahalpara, Bhatt and Sahu [7]. We use this in all our calculations.

For the present brief discussion we confine ourselves to axially symmetric prolate HF solutions. A more complete calculation, including oblate shapes also will be presented elsewhere. The single particle spectra corresponding to the lowest energy intrinsic HF state for ^{71}Br, ^{73}Br and ^{75}Br are shown in Figure 1. This defines our DSM. We can generate several excited configurations by taking particle-hole excitations over this ground-state configuration as described earlier. For N = 36, 38 we have considered all configurations in which the protons are either in $1/2^-$ or $3/2^-$ states and neutrons occupy either only *fp* orbits or two neutrons are in $1/2^+$ or $3/2^+$ states. This also includes rotation-aligned neutron configurations with $K = 1^+$. For N = 40 even the ground state configuration has two neutrons in $g_{9/2}$ state, and hence we consider excited configurations with 2 or 4 neutrons arranged in $1/2^+$ and $3/2^+$ states. For positive parity states, the proton is excited to the $1/2^+$ or $3/2^+$ state, with neutron in various configurations as for negative parity states. Full scale band-mixing calculations are carried out as described previously. Figures 2a–2c give the comparison between observed and calculated results.

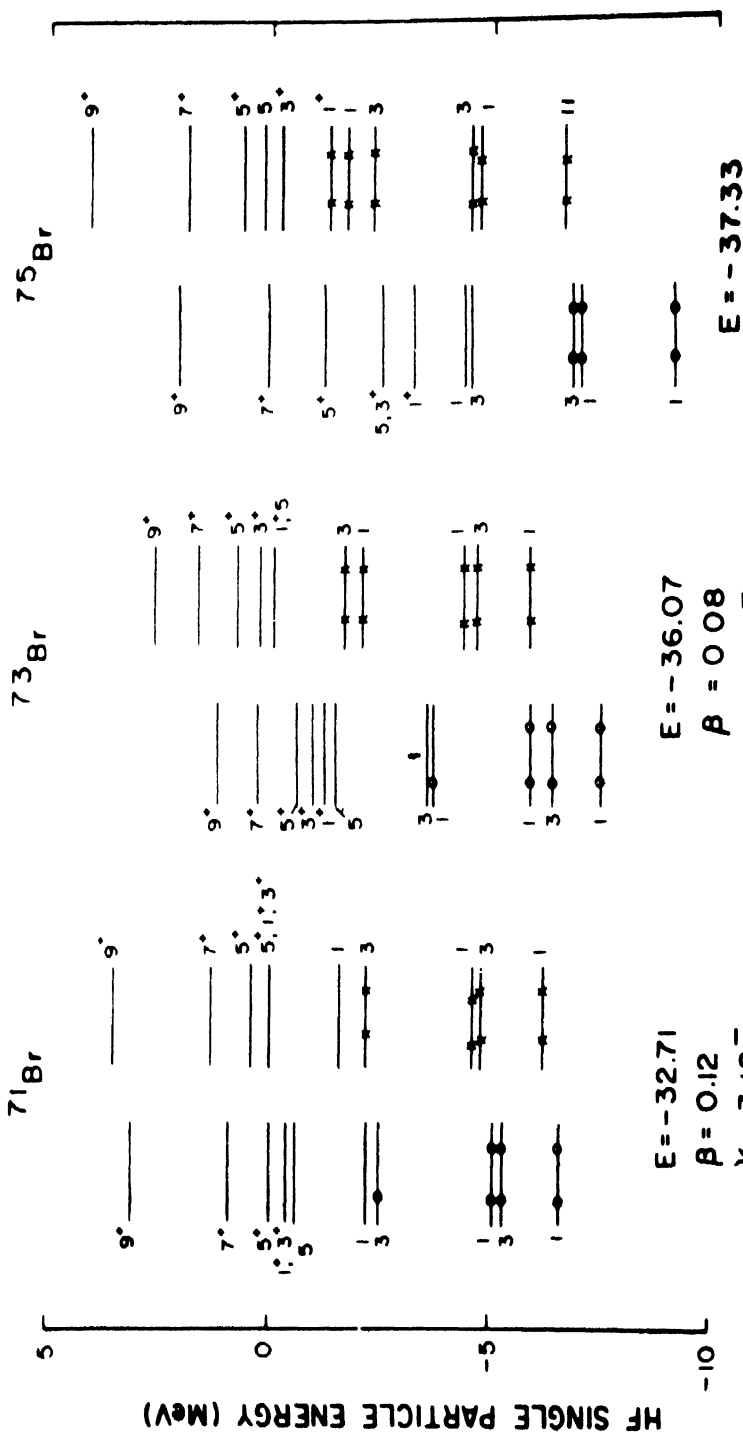

Figure 1. Single particle spectrum for the lowest energy intrinsic state given by HF calculations. The numbers next to levels denote 2k values. Protons are represented by circles and neutrons by crosses. The HF energy in MeV and the deformation parameter beta are also shown.

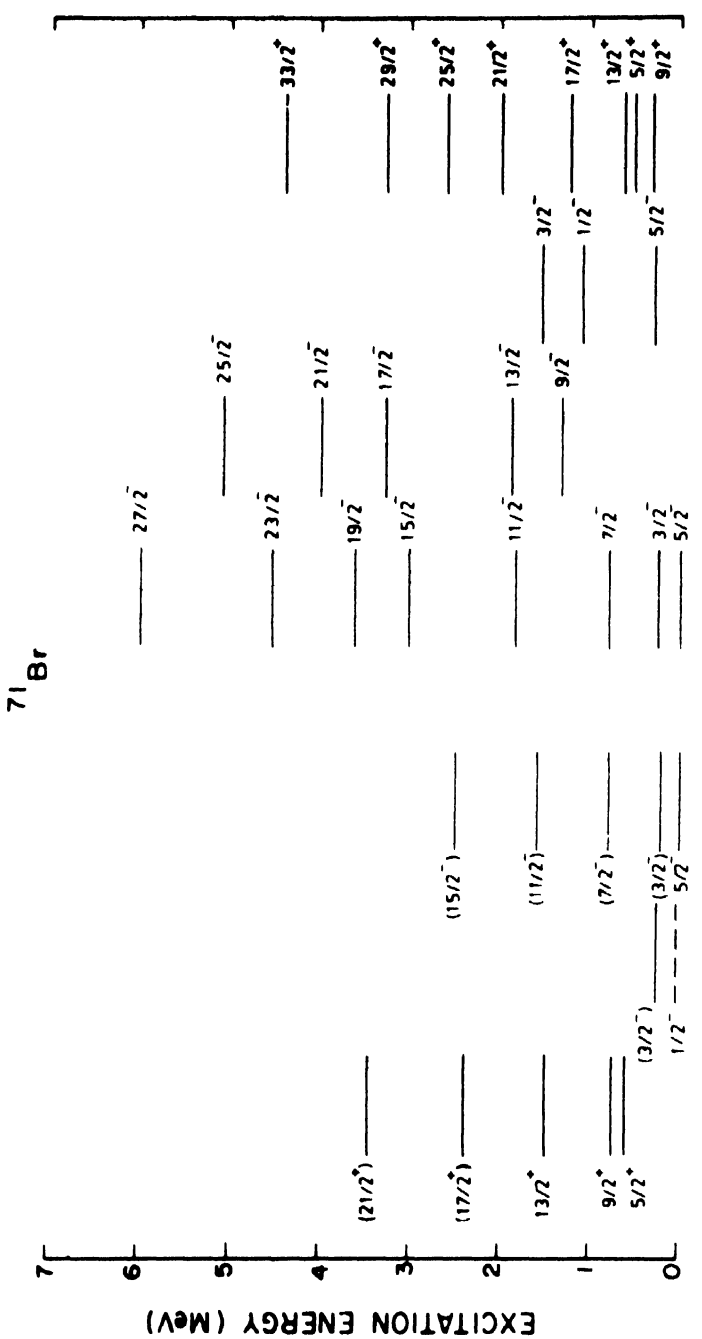

Figure 2a. Various collective bands of good J states obtained from DSM calculations compared to experimental data ^{71}Br

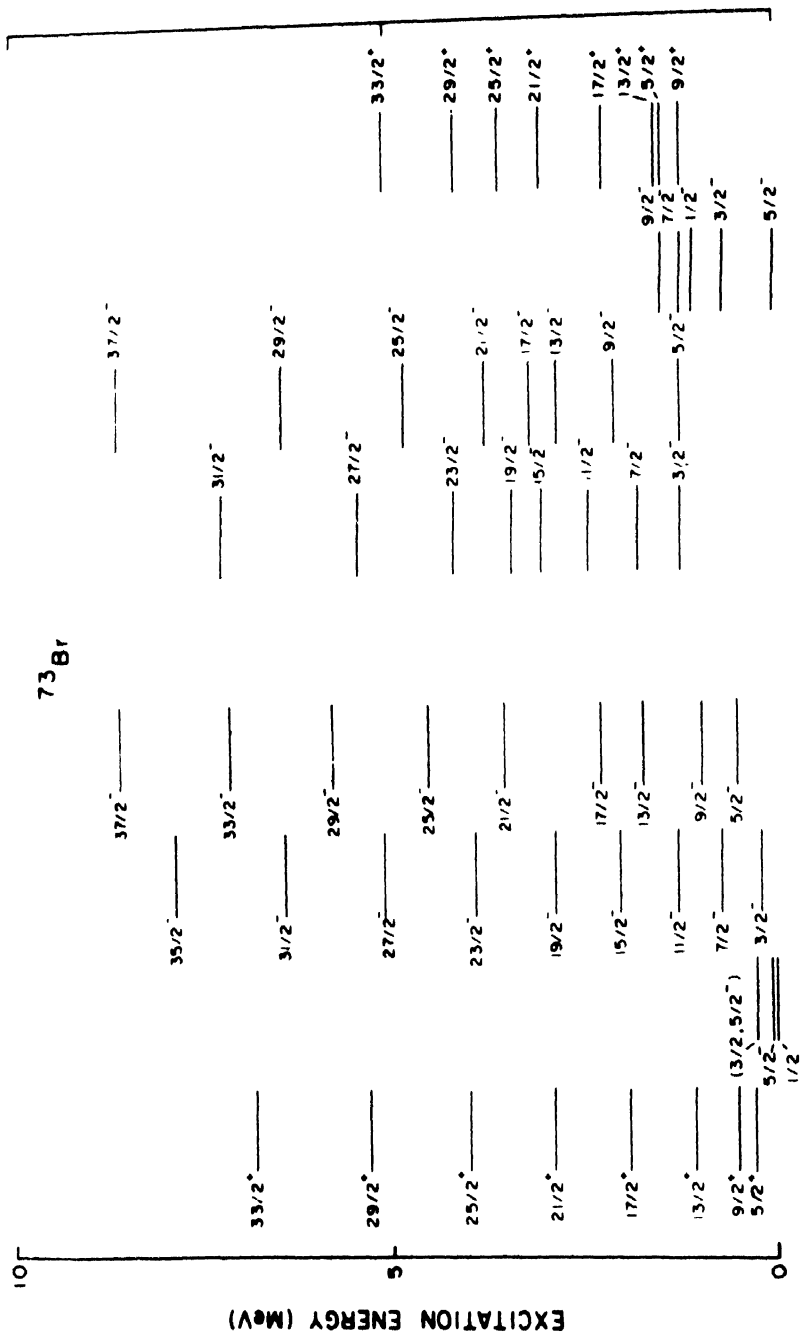

Figure 2b. Various collective bands of good J states obtained from DSM calculations compared to experimental data. ^{73}Br.

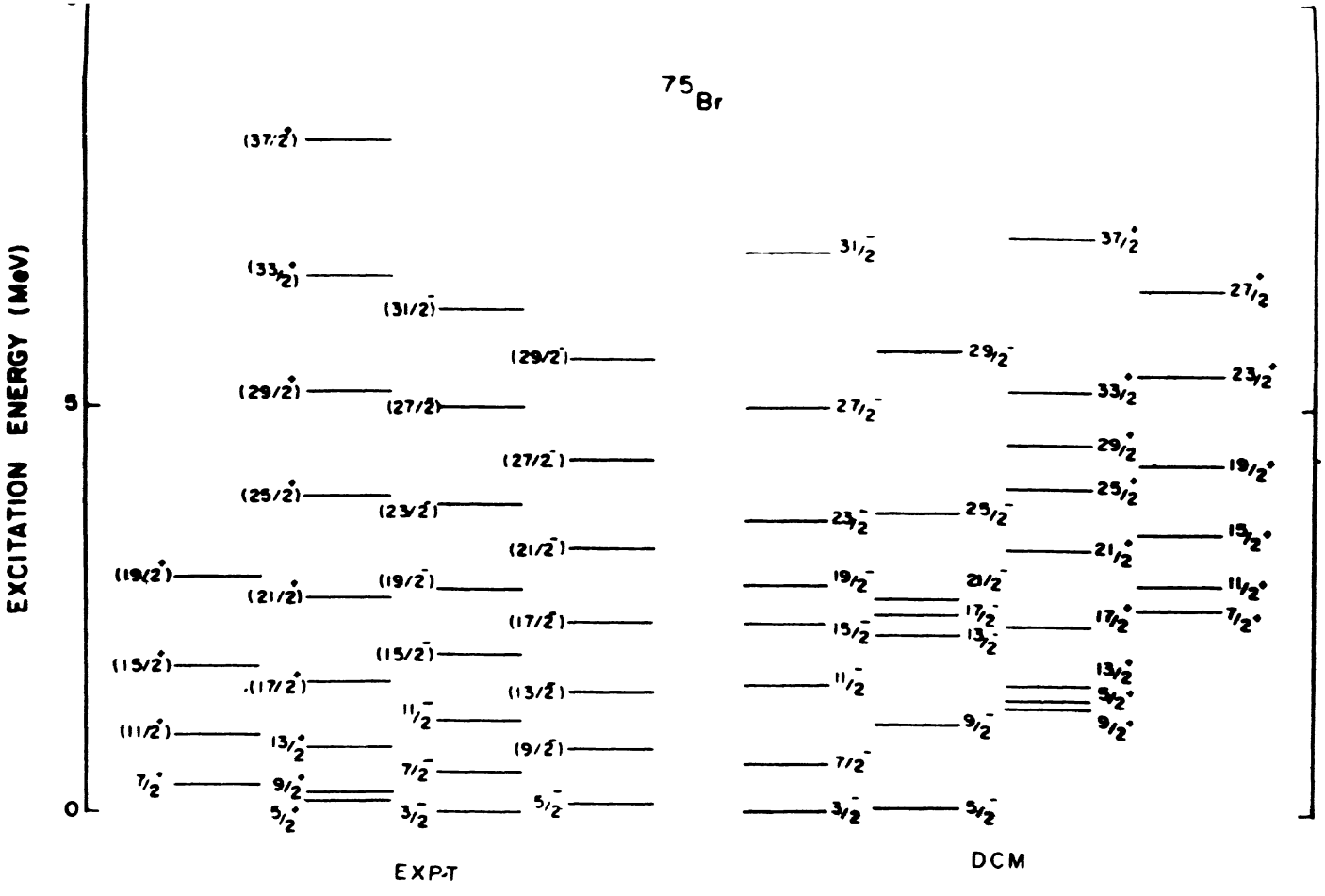

Figure 2c. Various collective bands of good J states obtained from DSM calculations compared to experimental data ^{75}Br

We shall only discuss some broad features of these spectra. The experiments show [14] in all three nuclei a well developed band of negative parity states based on a $K = 3/2^-$ state. For ^{71}Br and ^{73}Br, the $J = 5/2^-$ state of this band occurs below band head $J = 3/2^-$, and for ^{75}Br, the $J = 5/2^-$ is slightly above the $J = 3/2^-$ state, ^{71}Br and ^{73}Br show a $J = 1/2^-$ state nearly degenerate with $J = 5/2^-$ state, but this is not seen in ^{75}Br. The unfavoured branch of the $K = 3/2$ band is not yet seen in ^{71}Br. For all three nuclei we find in our calculations a well developed rotational yrast band with $J = 3/2^-$ ground state for ^{75}Br and $J = 5/2^-$ as ground state for ^{71}Br and ^{73}Br.

The experiments also show in all three nuclei a positive parity band beginning with $J = 5/2^+$ with a $J = 9/2^+$ very close in energy. Our calculations also show a similar band with $J = 9/2^+$ as the lowest state but $J = 5/2^+$ just above it. All the states of the band with $J > 13/2^+$ are quite well reproduced.

Analysis of the dynamic moment-of-inertia for ^{73}Br and ^{75}Br shows for positive parity states a band-crossing due to neutron alignment in $g_{9/2}$ state. Our calculations also show a similar alignment around $J = 25/2^+$ in both these nuclei. We also predict a similar band crossing at $J = 25/2^+$ in ^{71}Br. For the negative parity band, a similar analysis of experiments suggests the existence of two band crossings, the first one due to proton alignment, and the second one due to neutron alignment. However, our HF calculations show that to excite two protons from *pf* to *g* state would require much higher energy compared to that for two neutrons. Thus, whereas we do obtain a band crossing for two neutron alignment around $J = 19/2^-$ in these three nuclei, no such proton alignment seems possible in our model at low spins.

5. Conclusions

Our primary theme is that a Hartree-Fock calculation in a limited shell model configuration space generates a self-consistent deformed shell model basis. Configuration mixing calculations in this deformed shell model space provide a close approximation to standard spherical shell model calculations with a striking economy of computational labour. In fact DSM approach enables us to describe in a shell model framework a large number of nuclei that otherwise could not be calculated at all in spherical basis. Collective features of nuclear spectra at once become obvious and transparent. An application of DSM to proton-rich bromine nuclei is discussed.

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